02. CHEMBIOINFO-08: Cheminfo., Chemom., Bioinfo., Comput. & Quantum Chem. Congress München, GR-Cambridge, UK-Ch. Hill, USA, 2022.

Welcome Message

Dear colleagues worldwide welcome to a joint call of CHEMBIOINFO-08: Cheminformatics, Chemometrics, Bioinformatics, Computational & Quantum Chemistry Congress **München, Germany-Cambridge, UK-Chapel Hill, USA, 2022** . CHEMBIONFO is an inter-university trans-Atlantic Chem-Bioinformatics, Computational Chemistry, and Computational Biology congress series. From the America's side the event is organized by professors of University of North Carolina (**UNC Chape Hill**), Chape Hill, NC, **USA**, and professors of North Carolina Central University (**NCCU**), Durham, NC, **USA**. From Europe's side the event is organized by professors and researchers of Helmholtz Zentrum München - German Research Center for Environmental Health (**GmbH**), **Germany**, The European Bioinformatics Institute (**EMBL-EBI**), Cambridge, **United Kingdom**, Center for Neuroscience and Cell Biology (**CNC**), University of Coimbra (**UC**), Coimbra, Portugal, the University of The Basque Country (**UPV/EHU**) and **IKERBASQUE**, Basque Foundation for Science, Bilbao, **Basque Country, Spain**. This congress is associated to the **MOL2NET** International Conference Series on Multidisciplinary Sciences. MOL2NET (From Molecules to Networks), International Conference on Multidisciplinary Sciences, **ISSN**: 2624-5078, MDPI SciForum, Basel, Switzerland.

Topics of Interest. CHEMBIOINFO series aims to bring together leading academics, researchers and scholars to share their experiences on all aspects of computational programing, modeling, simulations, or scientific computing dedicated to Computational Chemistry, Chemoinformatics, Bioinformatics, Systems Biology, Biocomputing, etc. We focus on applications to Medicinal Chemistry, Drug Design & Discovery, Pharmaceutical Industry, Natural Products Research, Toxicology, Vaccine Design, Biotechnology, Personalized Medicine, Biomedical Engineering, etc. We welcome contributions involving the following topic:

Chemoinformatics & Computational Chemistry. Chemoinformatics, QSAR, QSPR, QSTR Modelling, Quantum Chemistry, Functional Density Theory (DFT), Ab Initio Methods, Semi-Empirical Methods, Machine Learning (ML) Quantum Chemistry Potentials, Molecular Mechanics/Molecular Dynamics (MM/MD), Molecular Docking, etc.

Chemometrics and Data Analysis. Chemometrics, Matlab, R and Python. Data types, PCA, Data Pre-processing, Multivariate Regression, Multivariate Classification, Variable selection methods, Multivariate Curve Resolution (MCR), Multi-way analysis, Non-linear modelling, Multiblock analysis and data fusion, Multivariate Error estimation, Design of Experiments, ANOVA-Simultaneous Component Analysis, Hyperspectral Image Analysis, Metabolomics Data Analysis.

Bioinformatics and Systems Biology. Proteomics, Genomics, BLAST and sequence alignment, Meta-Genomics, Protein folding and Protein Structure prediction, RNA secondary structure prediction, Protein Interaction Networks (PINS), Gene Regulatory Networks (GRN), Metabolomics and Metabolic Networks, Synthetic Biology, Data Analysis, and related techniques.

Computer Coding, Data Analysis, Artificial Intelligence, and Soft Computing. The congress also deals with the development or application of computer languages, computational programs, and/or algorithms for the study of chemical and biological process and/or inspired on biological processes. This include programing in Python/Biopython, Perl/Bioperl, etc. Development or application of Machine Learning (ML), Artificial Neural Networks (ANN), Deep Learning Networks (DLN), Bayesian Networks, Random Forest, Classification Trees, Genetic Algorithms (GA), Swarm Intelligence (SI), Ant Colony Algorithms, Artificial Imune Systems, etc.

Bioethics and Biolaw: Last, not the least, the workshop deals with all the Legal, Regulatory, and Bioethics issues emerging from use of new experimental and ICTs in the previous areas such as Drug patenting, Genome patenting, Drug re-purposing patents, Copyrights and Intellectual Property Protection of Cheminformatics, Chemometrics, Bioinformatics, and Computational Chemistry Software and Models, etc. GDPR and Personal data protection in Human Bioinformatics, etc.

CHEMBIONFO Associated Schools & Workshops

USINEWS-05: US-IN-EU Workshop Series in Chemoinformatics

UNIVERSITY OF MINNESOTA DULUTH

Driven to Discover℠

CHEMBIOIFO Congress will be one year more the online host of the dual call with associate workshops USINEWS-05: US-IN-EU Workshop Series in Chemoinformatics and IUWMC-08: Eighth Indo-US Workshop on Mathematical Chemistry. The historic roots of USINEWS workshop series are in the earlier versions of IUWMC founded and organized by Dr. **Suhbash C. Basak** during many years, as example of multicultural melting pot devoted to promote interdisciplinary collaborations in science. The works on this initiative started in 1990; the first event was organized in 1998 at Visva Bharati University, West Bengal, India. The Lecture Series was mainly to train young scholars. The third line of events was geared to benefit the South American scientists and young scholars. Two events have been held in Colombia. Some reports of these workshops are: *[J. Chem. Inf. Comput. Sci.*, 1999, 39 (2), pp 179–179], [*J. Chem. Inf. Comput. Sci.*, 2001, 41 (3), pp 479–479], *[J. Chem. Inf. Model.*,2006, 46 (1), pp 1-1]. These workshops included: (1) Indo-US Workshop on Mathematical Chemistry Series, beginning in 1998 in India and having six more events both in USA and India. (2) Indo-US Lecture Series on Discrete Mathematical Chemistry, four events mainly focusing on the training of young scholars. (3) Mathematical Chemistry Workshops of the Americas (involving countries of North and South Americas).

More recently, USINEWS workshops series have been co-founded by its honor chairman Prof Dr. **Suhbash C. Basak**, University of Minnesota, **Duluth, USA** , Prof. **Danail Bonchev**, Center for the Study of Biological Complexity, Virginia Commonwealth University (VCU), Richmond, **USA**, and Prof. **González-Díaz H**., MOL2NET Founder Chairman, IKERBASQUE Professor, Dept. of Org. & Inorg. Chem., BIOFISIKA UPV/EHU-CSIC Institute, University of the Basque Country UPV/EHU, and IKERBASQUE, Basque Foundation for Science, **Basque Country, Spain.** USINEWS have been and/or is currently also co-chaired before by Dr. **Shameer Khader**, Philips Healthcare, Cambridge, MA, USA, Prof. **Ashok. K. Dubey**, NSIT Netaji Subhas Institute of Technology, New Delhi, India, Prof. **Kunal Roy**, Jadavpur University, **India.**

USINEWS series have been devoted to attract communications and foster collaborations in Chemoinformatics between USA, Europe, and India researchers worldwide. USINEWS has served also as the mirror workshop of IUWMC in MOL2NET Conference. Consequently, USINEWS have accepts both direct publications and summaries of IUWMC works. USINEWS/IUWMC series have been published by MOL2NET conference in SCIForum platform as standalone congresses/workshops see **USINEWS-04**, **USINEWS-03** congresses. USINEWS/IUWMC communications or summaries have been published also by MOL2NET series as associated workshops of the **CHEMBIOINFO-04** congress (see **USINEWS-02** associated workshop) or **USEDAT-03** congress (see **USINEWS-01** associated workshop).

Topics. IUWMC-08/USINEWS-05 will focus on emerging topics at the interface of mathematical and computational chemistry as well as their applications in the emerging fields of Chemoinformatics, Bioinformatics (including genomics, vaccinomics & proteomics), ecotoxicology, quantitative structure-activity relationship (QSAR), quantitative molecular similarity analysis (QMSA), and other relevant fields. This is the official page of **IUWMC-08** (click on the acronym).

IUWMC-08 Themes. Theme I: Mathematical characterization of molecular & biomolecular structure. Theme II: Applications of mathematical chemistry to quantitative structure-activity relationship (QSAR), quantitative molecular similarity analyses (QMSA), molecular design & new drug discovery. Theme III: Applications of mathematical chemistry to genomics, proteomics, vaccinomics & computational biology. Theme IV: Applications of mathematical chemistry to environmental toxicology and regulation of chemicals.

IUWMC-08 Objectives. 1. To review the progress in the field of mathematical chemistry and its applications. 2. To bring together scientists, scholars, and students together for an effective interaction among them, aimed at sharing their knowledge and experience concerning basic and applied research in this emerging field.

CHEMBIOINFO, IUWMC, & USINEWS, Modalities of Participation. The congress series may run both in person and/or online depending on year. Participation in all modalities is not mandatory. Online/person presentations may include workshops, seminars, meetings with face-to-face discussion at both universities and/or online publication of papers, videos, etc.

CHEMBIOINFO, IUWMC, & USINEWS, Online publication. This congress will be hosted online by the MOL2NET conference series. It means, that all communications will be published online at Sciforum platform. All presentations will be published in **open access** and a **DOI number will be assigned**. This include, conference papers, letters,, posters, etc. The platform also includes the possibility of online comments from researchers of both universities and colleagues worldwide as well.

CHEMBIOINFO Online Publication Steps: As this joint pursuit to increasing the interactions between CHEMBIOIFO community with all other Mol2Net conference participants and also with researchers worldwide we split the congress on two main stages. In 1st stage called Publication stage the participants will submit, upload, and publish their communications. In the 2nd stage, called Post-publication discussions, the participants will post comments or questions in the papers of other authors and/or answer to comments made by others about their own works. The steps to are the following:

CHEMBIOINFO Publication stages

(00) Register, Sign in/Login, to Sciforum platform **[Sciforum login]**
(01) Submit the title/abstract to workshop (do not upload paper here)
(02) Download template doc and prepare your communication
(03) Wait for Sciforum abstract acceptance email
(04) Follow the link in the email or login to upload paper (doc and pdf format)

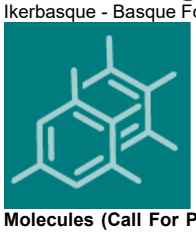
CHEMBIOINFO Post-publication stage

(05) Wait for paper acceptance and publication emails
(06) Follow link to proofread your paper
(07) Communicate with chairpersons if corrections are necessary
(08) Wait for advice of post-publication season starting
(09) Login to post comments, questions, or answer comments about your work
(10) Request author (publication) and/or reviewer (post) attendance certificate.

MDPI JCR Journals Special Issues

In parallel, the members of committees and/or authors are encouraged to edit special issues for different journals of the editorial MDPI (http://www.mdpi.com/). The special issues run in parallel, or totally independently from the conference. Manuscripts should be submitted online at www.mdpi.com by registering and logging in to this website. In order to send a proposal of associated workshop and/or special issue contact the chairperson of the conference Prof. González-Díaz H. Please, check the following special issues associated to the topic of the workshop.

IJMS (Call For Papers): Special Issue: **Complex Networks, Bio-Molecular Systems, and Machine Learning 2.0**. Journal: International Journal of Molecular Sciences IJMS (ISSN 1422-0067), **JCR IF = 6.208**. Topics: Chemoinformatics, Bioinformatics, QSAR/QSPR Models, Molecular descriptors, Graph Theory, Complex Networks, Protein Interaction Networks, Metabolic Networks, Machine Learning, Artificial Neural Networks (ANN), Deep Learning, Software development, Guest Editor: **Prof. Humberto González-Díaz**, Email: mol2net.chair@gmail.com, Department of Organic and Inorganic Chemistry, and Basque Center for Biophysics, University of the Basque Country (UPV/EHU) and Ikerbasque - Basque Foundation for Science, 48011 Bilbao, Biscay, **Spain**. Submissions until: **2023-Feb-28**.



Molecules (Call For Papers): Special Issue: **QSAR and QSPR: Recent Developments and Applications III.** Journal: ***Molecules*** (ISSN 1420-3049), **JCR IF = 4.411**. Topics: QSAR/QSPR modelling, Development of molecular descriptors, Molecular structure representation, Data mining, Machine learning. Editors: Dr. **Bono Lučić**, Rudjer Bošković Institute, NMR Centre, **Zagreb, Croatia**, **Prof. Bakhtiyor Rasulev**, Department of Coatings and Polymeric Material, **Fargo, USA**. Submissions Until: **2022-Dec-15.**

Antibiotics (Call For Papers): Special Issue: **Computational Approaches in Discovery & Design of Antimicrobial Peptides**. Journal: **Antibiotics** (ISSN 2079-6382), **JCR IF = 4.639**. Topics: Rational search and design of AMPs, Alignment-based and alignment-free approaches, Machine learning, Artificial intelligence, Biodiscovery with associated computational analyses/tools, Non-conventional in silico approaches, Guest Editors: Prof. **Agostinho Antunes**, Interdisciplinary Centre of Marine and Environmental Research (CIIMAR), Rua dos Bragas, 289, 4050-123 Porto, Portugal. Dr. **Guillermin Agüero**, CIIMAR, Interdisciplinary Centre of Marine and Environmental Research, University of Porto, **Portugal**. Email: gchapin@ciimar.up.pt. Prof. Dr. **Yovani Marrero-Ponce**, University San Francisco de Quito (USFQ), Quito, 170157, Pichincha, **Ecuador**. Submissions until: **2022-Dec-31**.

IJMS (Published): Special Issue: **Artificial Intelligence and Machine Learning in Drug Development**. Journal: International Journal of Molecular Sciences IJMS (ISSN 1422-0067), **JCR IF = 5.924**. Editor: Editor: Dr. **Irina Moreira**, Center for Neuroscience and Cell Biology (CNC), University of Coimbra, **Coimbra, Portugal**. Email: irina.moreira@cnc.uc.pt. Submissions until: **30 April 2022**.

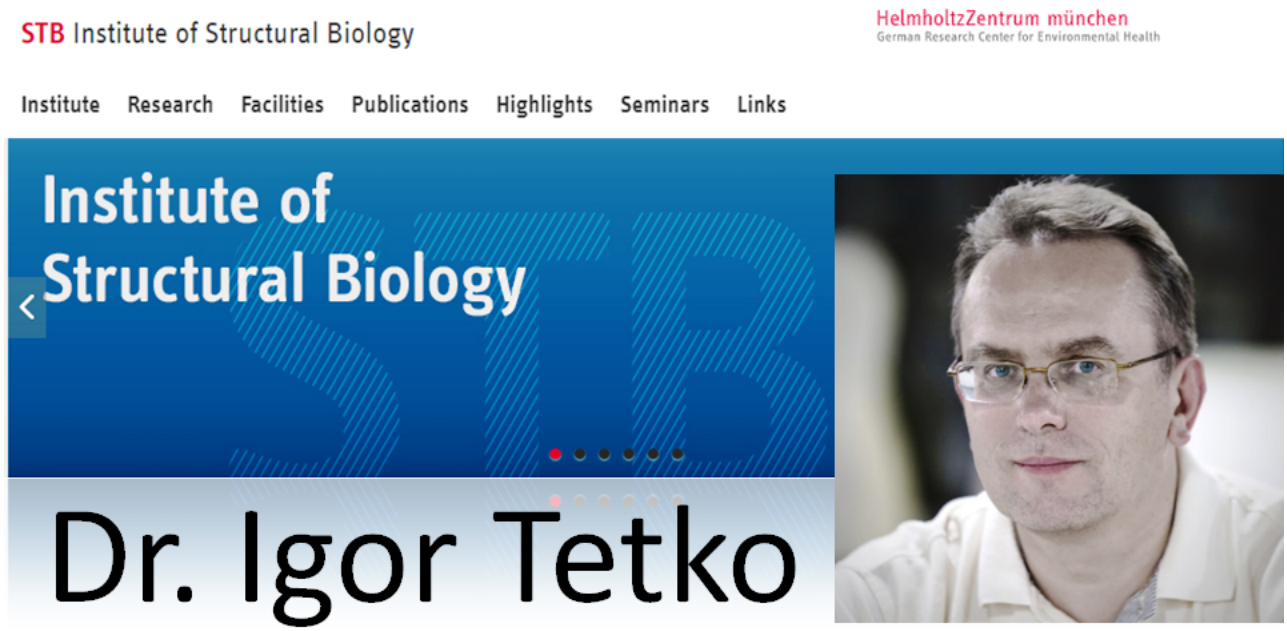
IJMS (Published): Special Issue: **Complex Networks, Bio-Molecular Systems, and Machine Learning**. Journal: International Journal of Molecular Sciences IJMS (ISSN 1422-0067), **JCR IF = 5.924**. Editor: **Prof. Humberto González-Díaz**, Email: mol2net.chair@gmail.com, Department of Organic and Inorganic Chemistry, and Basque Center for Biophysics, University of the Basque Country (UPV/EHU) and Ikerbasque - Basque Foundation for Science, 48011 Bilbao, Biscay, **Spain**. Submissions until: **28 Feb 2022**.

IJMS (Published): Special Issue: **Artificial Intelligence in Drug Discovery: Search, Data and Text Mining, Analytics, and Visualization**. Journal: **International Journal of Molecular Sciences** IJMS (ISSN 1422-0067), **JCR IF = 4.556**. Topics: Chemoinformatics, Quantitative Structure-Activity/Property Relationship QSAR/QSPR, Computational chemistry, Machine Learning, Transformers, Guest Editor: **Dr. Igor V. Tetko**, Helmholtz Zentrum Muenchen - German Research Center for Environmental Health and BIGCHEM GmbH, **Neuherberg, Germany**. Closed: **2021-Ago-31**.

CHEMBIOINFO USA Co-Host Honor Chairman

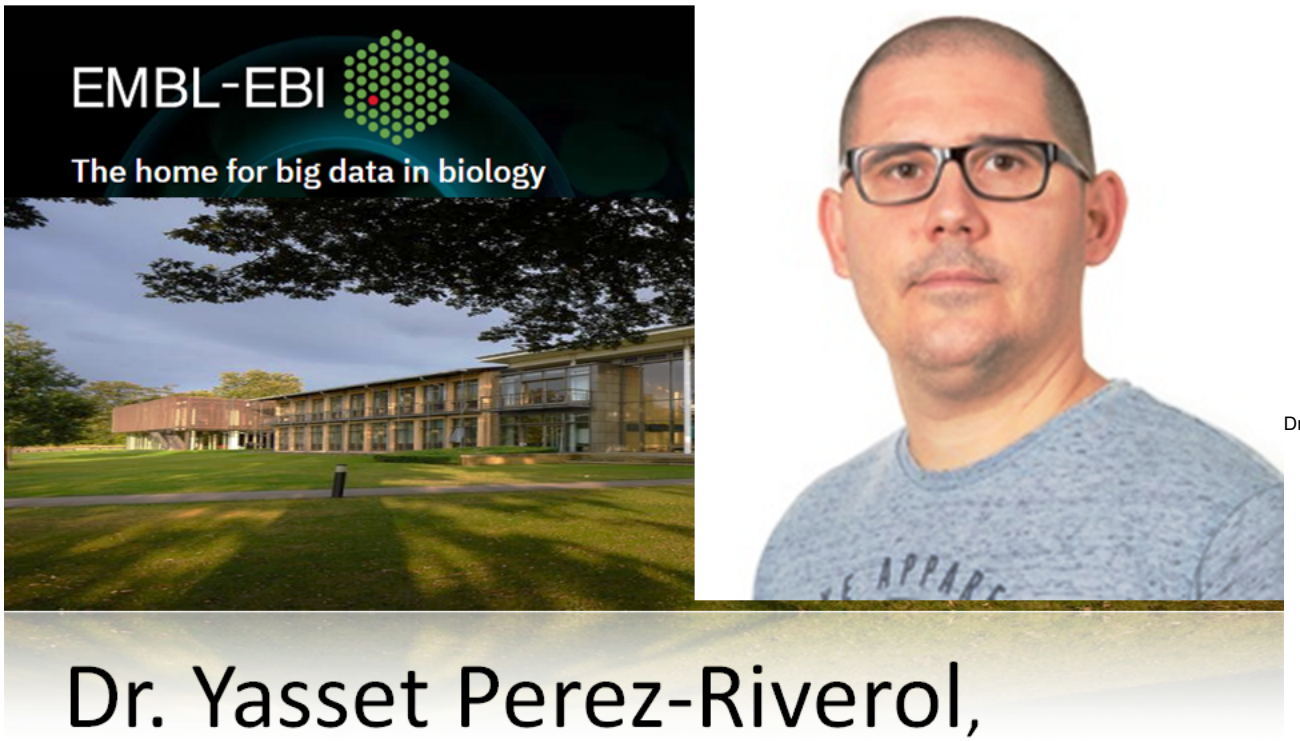
Prof. **Alexander Tropsha**, Associated Dean UNC Eshelman School of Pharmacy, Associated Editor J. Chem. Info. Model., ACS, USA. University of North Carolina , Chapel Hill, 27599, **North Carolina, USA**. Email: **alex_tropsha@unc.edu**

CHEMBIOINFO GERMANY Co-Host Honor Chairman



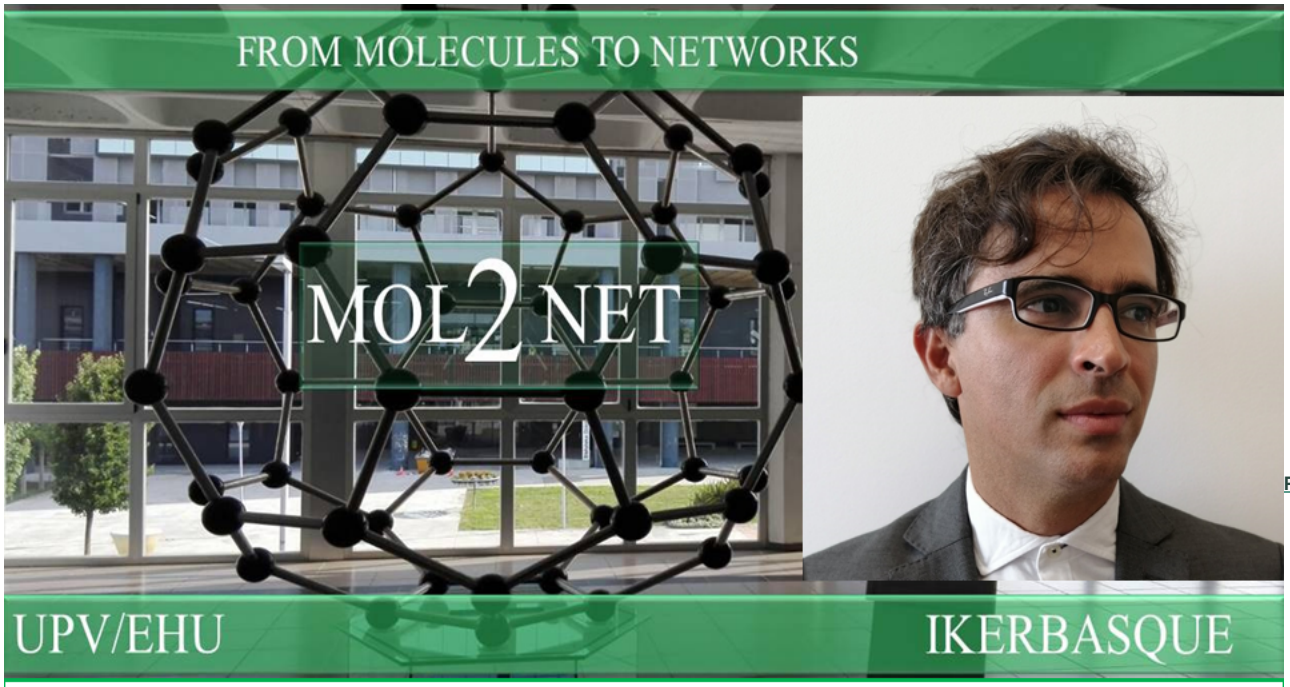
Dr. **Igor Tetko**, Inst. of Struct. Biol., Helmholtz Zentrum München - German Research Center for Environmental Health (GmbH), Neuherberg, **Germany.** Email: **i.tetko@helmholtz-muenchen.de**

CHEMBIOINFO UK Co-Host Honor Chairman



Dr. **Yasset Perez-Riverol**, European Bioinformatics Institute(EMBL-EBI), **Cambridge, United Kingdom**.

CHEMBIOINFO Series Founder Steering Chairman



Prof. Humbert González-Díaz

MOL2NET & USEDAT Chairman

UPV/EHU, **IKERBASQUE**, Basque Foundation for Science

Email (Direct Submission): mol2net.chair@gmail.com

SCAN ORCID QR

González-Díaz, **IKERBASQUE Professor, Email:** mol2net.chair@gmail.com,
(1) Dept. of Organic Chemistry II, University of the Basque Country UPV/EHU , 48940, Leioa, Biscay, Spain.
(2) IKERBASQUE, Basque Foundation for Science , 48011, Bilbao, Biscay, Spain.
ORCID: https://orcid.org/0000-0002-9392-2797

CHEMBIOINFO-07 Dedicated to Prof. Grammatica

Prof. Paola Gramatica
Full professor of Environmental Chemistry
Faculty of Sciences, Insubria University, Italy

Prof. **Paola Gramatica**, Full professor of Environmental Chemistry, Faculty of Sciences, Insubria University, **Italy**.
Email: **paola.gramatica@uninsubria.it**

CHEMBIOINFO-06 Dedicated to Prof. Todeschini

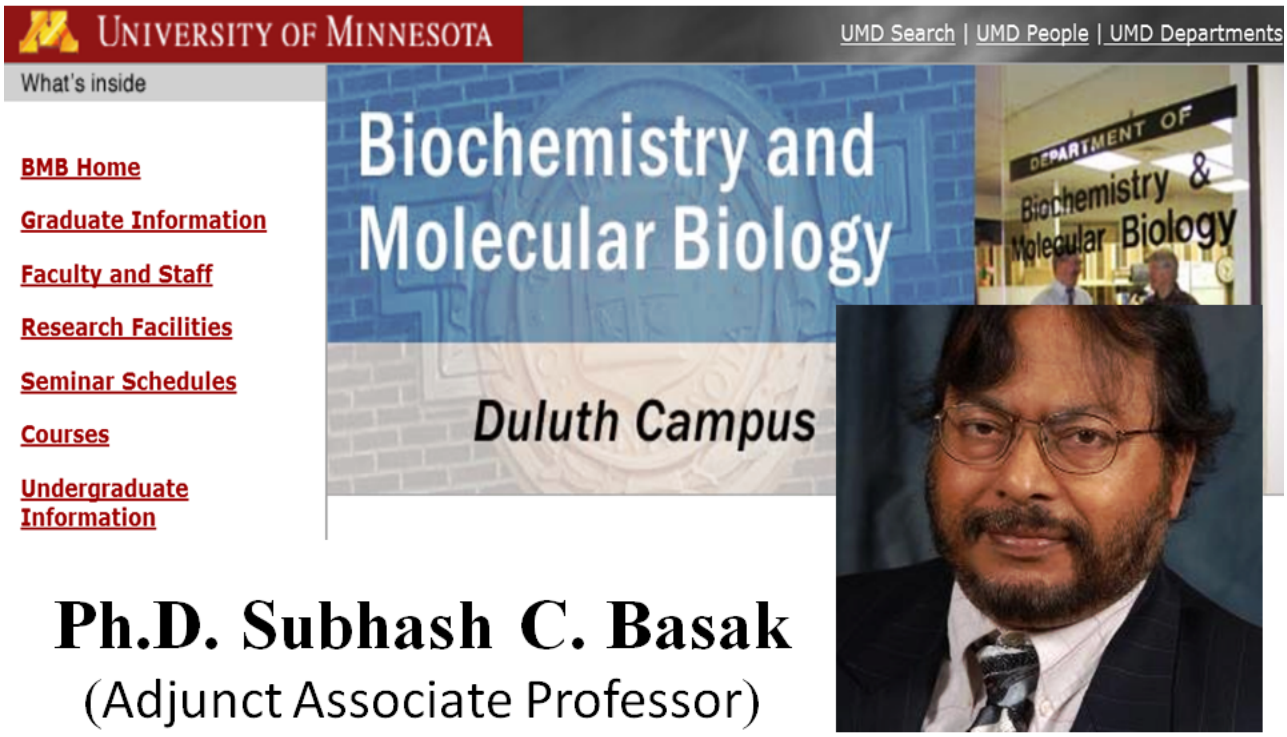
Prof. Roberto Todeschini, Department of Environmental Sciences, University of Milano-Bicocca, Milano,Italy.

CHEMBIOINFO-06 Dedicated to Prof. Bonchev

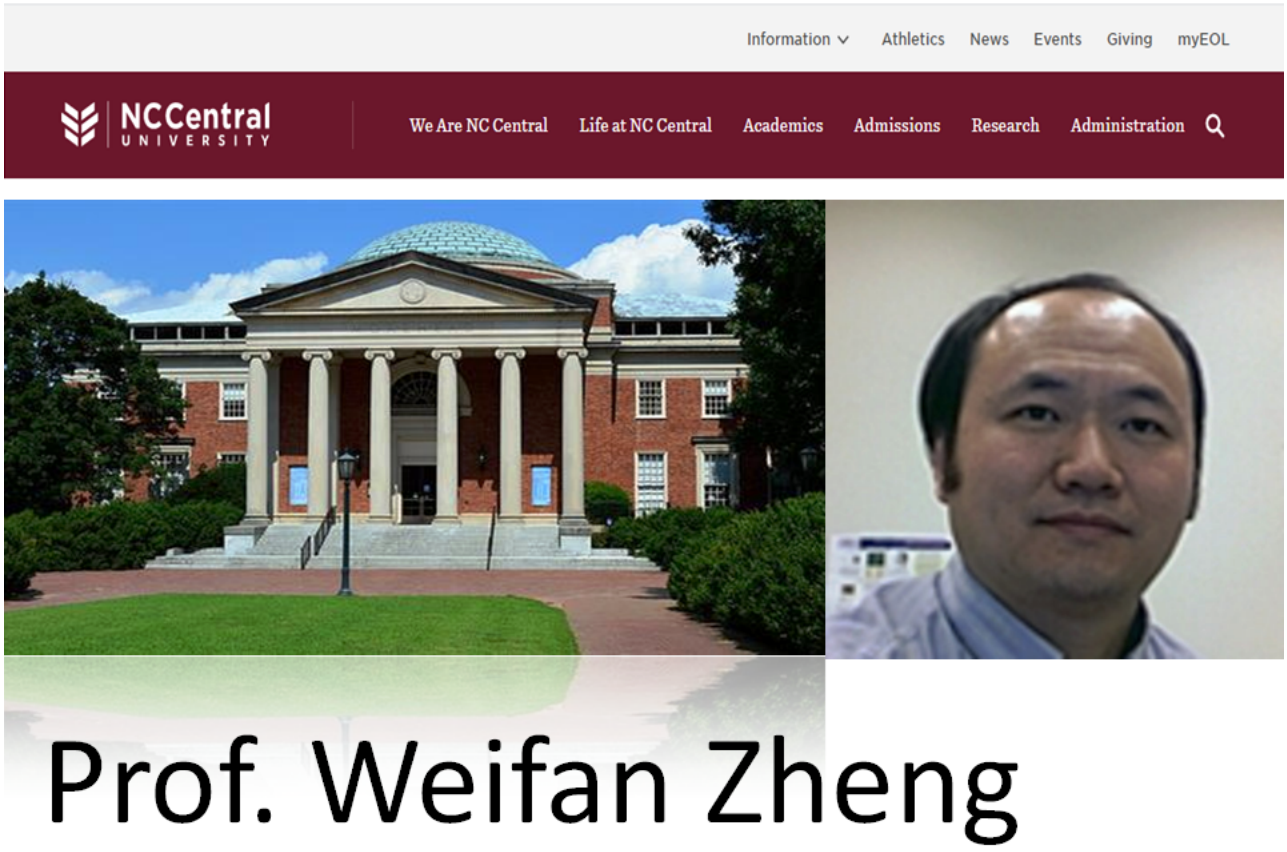
Prof. Danail Bonchev

Prof. Danail Bonchev, Center for the Study of Biological Complexity, Virginia Commonwealth University (VCU), Richmond, **USA**.
CHEMBIOINFO-08 Honor Advisory Scientific Committee

Prof. **Stephan Schürer**, Miller School of Medicine, Dept. of Molecular and Cellular Pharmacology, and Sylvester Comprehensive Cancer Center, University of Miami School of Medicine, **Miami, FL, USA**. Email: **sschurer@miami.edu**



Prof. Dr. Subhash C. Basak, Senior Scientist and Adjunct Assoc. Prof., Dept. of Chemistry, University of Minnesota Twin Cities, MN, **USA**. (CHEMBIOINFO Co-chairman, USINEWS & IUWMC Chairman)



Prof. Weifan Zheng, Department of Pharmaceutical Sciences, North Carolina Central University, **Durham, USA**.
Email: wzheng@nccu.edu

Prof. Dr. Irina Moreira, Center for Neuroscience and Cell Biology (CNC), University of Coimbra, Coimbra, **Portugal.**
Founder Chairperson of Series Meeting of Young Researchers in Structural Computational Biology (EJIBCE),
See last editions (EJIBCE 2018), (EJIBCE 2017), Emails: irina.moreira@cnc.uc.pt

ikerbasque
Basque Foundation for Science

Sobre nosotros Convocatorias Investigadoras/es Noticias Intrar

Prof. Jose Manuel Amig

IKERBASQUE Prof.

Prof. **Jose M. Amigo Rubio**, Dept. of Analytical Chemistry, University of Basque Country UPV/EHU, Leioa, **Basque Country, Spain.**

UNC | ESHELMAN SCHOOL OF PHARMACY

About Academics Research Divisions Faculty News Events Alumni

Eugene Muratov, Ph.D.

ASSOCIATE DIRECTOR, MOLECULAR MODELING LAB
RESEARCH ASSOCIATE PROFESSOR

Prof. **Eugene Muratov**, Laboratory for Molecular Modeling, UNC Eshelman School of Pharmacy, University of North Carolina , Chapel Hill , North Carolina 27599 , **USA**. Email: **murik@email.unc.edu**

CHEMBIOINFO-08 Scientific Committee
Dr. **Vincent Blay Roger**, Biol. Syst. & Eng. Division, Lawrence Berkeley National Laboratory, **Berkeley, CA, USA**.
Prof. **Bakhtiyor Rasulev**, Dept. Coat. & Polym. Mat., North Dakota State University (NDSU), **Fargo, ND, USA**.
Dr. **Subhash C. Basak**, Dept. of Chemistry and Biochemistry, University of Minnesota, **Duluth, MN, USA**.
Prof. **Robersy Sánches**, Eberly College of Science, Pennsylvania State University (PennState), **PA, USA**.
Prof. **Matthew M. Montemore**, Dept. Chem. & Biomol. Eng., Tulane University, **New Orleans, LA, USA**.
Prof. **Agostinho Antunes**, CIIMAR, Interdisc. Centre of Marine and Environ. Research, **Porto, Portugal**.
Dr. **Guillermin Agüero**, CIIMAR, Interdisc. Centre of Marine and Environ. Research, **Porto**, **Portugal**.
Prof. **Davide Ballabio**, Chemometrics Group, Università of Milano-Bicocca (UNIMIB), **Milano, Italy**.
Prof. **Jordi Mestres**, CEO ChemoTargets, IMIM, Univ. Pompeu Fabra, **Barcelona, Catalunya**, **Spain**.
Prof. **Natalia D.S. Cordeiro**, Dept. of Chem. and Biochem., University of Porto, **Porto, Portugal.**Dr. **Alla Toropova**, Istituto di Ricerche Farmacologiche Mario Negri, **Milano, Lombardy, Italy**.
Dr. **Andrey Toropov**, Istituto di Ricerche Farmacologiche Mario Negri, **Milano, Lombardy, Italy**.

CHEMBIOINFO Founder Steering Chairman
Prof. **González-Díaz H**., IKERBASQUE Professor, Email: mol2net.chair@gmail.com
(1) Dept. of Org. & Inorg. Chem., University of the Basque Country UPV/EHU, **Basque Country, Spain.**
(3) BIOFISIKA UPV/EHU-CSIC Institute, 48940, Leioa, Grt. Bilbao, **Basque Country, Spain.**
(2) IKERBASQUE, Basque Foundation for Science , 48011, **Bilbao, Basque Country, Spain**.

CHEMBIOINFO Assistant Chairperson
Prof. **Sonia Arrasate**, Email: sonia.arrasate@ehu.eus
Dept. Org. & Inorg. Chem., Univ. of Basque Country (UPV/EHU), **Basque Country, Spain.**

CHEMBIOINFO ICTs, Bioethics, & Regulatory Affairs Chairperson
Dr. **Aliuska Duardo-Sanchez** (Law.Lic., Ph.D. TICSs & Legal Sciences)
IKERDATA S.L. Data Protection Officer (DPO), ZITEK, Univ. of Basque Country (UPV/EHU),
Rectorate Building, Sarriena w/n, 48940, Leioa, Grt. Bilbao, **Basque Country, Spain.**

CHEMBIOINFO Registration Manager
MSc. **Harbil Bediaga**, IKERDATA S.L. CEO, University of The Basque Country UPV/EHU
ZITEK, Office 6, Rectorate Building, 48940, Leioa, Greater Bilbao, **Basque Country, Spain.**
Link: https://www.ikerdata.com/, Email: adm@ikerdata.com

CHEMBIOINFO Committee Assistant
MSc. **Andrea Ruiz Escudero**, IKERDATA S.L. INVESTIGO NextGenerationEU Researcher
University of The Basque Country UPV/EHU, ZITEK, Office 6, Rectorate Building,
Leioa, 48940, Greater Bilbao, Basque Country, Spain.
Link: https://www.ikerdata.com/, Email: ikerdata.andrearuiz@gmail.com

ongress Chair
rof. Dr. Sonia Arrasate Gil, Dept. Organic and Inorganic Chemistry, University of The Basque Country UPV/EHU, 48940, Leioa, Greater Bilbao, Basque Country, Spain.

Hide published submissions (23)

Submissions

List of Papers (23) Toggle list

Id	Title	Presentation Video	Presentation Pdf	Authors
sciforum-060723	**Activity prediction, toxicity and molecular modeling of terpenoids against tuberculosis**	N/A		Emille Da Silva, Paulo Pe Teresa Rodrigues, Jessica De Moura, Igor De Araujo, Jeremias Emídio, Marcus Scotti, Luciana Scotti, Alex Monteiro
sciforum-061289	**Applications of machine learning and artificial intelligence for Covid-19 (SARS-CoV-2) pandemic**	N/A	N/A	Maider Baltasar Marchu
sciforum-069051	**Artificial intelligence and machine learning in Leishmania drug discovery**	N/A	N/A	Gabriel Mazón-Ortiz, Galo Cerda-Mejía, Karel Diéguez-Santana Juan Ruso
sciforum-060448	**Bioinformatic tools for proteomic data analysis**	N/A		Luisa Chocarro, Ester Blanco, Hugo Ara , Leticia Fernández Rut Ana Bocanegra, Miriam Echaide, Maider Garnica, Pablo Ramos, Enrique Santamaría, Joaquín Fernández Irig , Grazyna Kochan, David Escors
sciforum-060721	**Computational study by molecular docking of structures from algae predicting activity against the protozoan Leishmaniasis donovani and toxicity parameters**	N/A		Paulo Pereira, Emille Da S Jeremias Emídio, Igor De Araujo, Jessica De Moura, Teresa Rodrigues, Marcus Scotti, Luciana , Alex Monteiro
sciforum-069038	Editorial: CHEMBIOINFO-08: Cheminfo., Chemom., Bioinfo., Comput. & Quantum Chem. Congress München, GR-Cambridge, UK-Ch. Hill, USA, 2022.	N/A	N/A	Humbert Díaz

Id	Title	Presentation Video	Presentation Pdf	Authors
sciforum-069279	Engineering protein fragments via evolutionary and protein-protein interaction algorithms: ***De novo*** design of peptide inhibitors for F_OF_1-ATP synthase	N/A	N/A	Yasser Ruiz-Blanco, Luis Ávila-Barrientos, Enrique Hernández-Garcí Guillermin Agüero-Chap Agostinho Antunes, Enrique García-Hernán
sciforum-068450	Identification of Natural Products with Potential Activity against ***Leishmania amazonensis*** using computational models and experimental corroboration	N/A	N/A	Naiví Flores-Balmaseda Ailin Ramírez-Abreu, Lianet Monzote, Niurka Mollineda, Sergio Sifontes-Rodrígue Juan Castillo-Garit
sciforum-062408	Immunoinformatic and genomic characterization of SARS-CoV-2 helicase (nsp13) mutational profile; an attractive antiviral therapeutic target	N/A	N/A	Niti Yashvardhini, Deepak Jha, Amit Kum Kumar Sayrav
sciforum-060737	Molecular docking study in silico of chemical constituents of ***Paubrasilia echinata*** Lam., against chagas disease	N/A		Igor De Araujo, Jessica De Moura, Teresa Rodrigues, Paulo Pereira, Jeremias Emídio, Emille Da Silva, Marcus Scotti, Luciana Scotti, Alex Monteiro
sciforum-069034	Post-publication cover of A Hybrid Machine Learning and Network Analysis Approach	N/A	N/A	Emiliano Giardina
sciforum-069039	Post-publication cover of Molecular Topology for the Search of New Anti-MRSA Compounds	N/A	N/A	Jose I. Bueso-Bordils
sciforum-069033	Post-publication notes of Rapid Discrimination of Neuromyelitis Optica Spectrum Disorder and Multiple Sclerosis	N/A	N/A	Nicolas Collongues, Youssef El Khoury
sciforum-069037	Post-publication summary of Hybrid Deep Learning Based on a Heterogeneous Network Profile	N/A	N/A	Kitiporn Plaimas
sciforum-069030	Post-publication summary of Identification of D Modification Sites Using a Random Forest Model	N/A	N/A	Liang Yu, Hong-Xia H
sciforum-069036	Post-publication synopsis of The Crosstalk between SARS-CoV-2 Infection and the RAA System	N/A	N/A	Piotr Formanowicz
sciforum-068449	Predicting Blood-Brain Barrier Passage using AWV and Machine Learning	N/A		Yoan Martínez López, Yanaima Jauriga Ortiz, Ansel Rodríguez Gonza Juan A. Castillo Garit, Gerardo M. Casanola-M , Julio Madera Quintana

Id	Title	Presentation Video	Presentation Pdf	Authors
sciforum-061317	**Prediction of antihistamine activity according to QSAR methods**	N/A	N/A	Luis Alberto Torres-Gor Melisa Gil Chavez, Ivon Gonzalez Blanco
sciforum-060725	**Prediction of antiviral activity, cytotoxicity risks and molecular docking against HIV of constituents from marine algae**	N/A		Teresa Rodrigues, Jessica De Moura, Igor De Araujo, Paulo Per Emille Da Silva, Jeremias Emídio, Marcus Scotti, Luciana Scotti, Alex Monteiro
sciforum-061404	**QSPR modeling of log p for drugs potentially active on the central nervous system**	N/A	N/A	Luis Alberto Torres-Gor Juan Carlos Polo, Alejandro Almeida Pons
sciforum-069153	**The application of Machine Learning to Raman spectroscopy**	N/A	N/A	Andrea Ruiz Escudero
sciforum-061019	**The potential applications of Artificial Intelligence in drug discovery and development**	N/A	N/A	Ane Ibáñez Antolín
sciforum-068327	**Virtual Screening Multitarget-Based Against 3CL^{pro} and TMPRSS2 Reveals New Promising Drugs Against SARS-CoV-2.**	N/A	N/A	Daniel Medeiros, Marianny De Souza, Ricardo de Moura, Igor Nascimento